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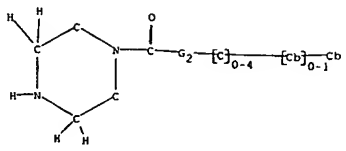

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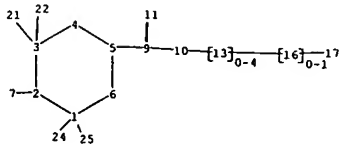

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7 9 10 11 13 16 17 21 22 24 25
ring nodes :
1 2 3 4 5 6
chain bonds :
1-24 1-25 2-7 3-21 3-22 5-9 9-10 9-11 10-13 13-16 16-17
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-9 9-10 9-11 10-13
exact bonds :
1-24 1-25 2-7 3-21 3-22 13-16 16-17
isolated ring systems :
containing 1 :

G1:H,CH3

G2:O,S

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 9:CLASS 10:CLASS 11:CLASS
13:CLASS 16:Atom 17:Atom 21:CLASS 22:CLASS 24:CLASS 25:CLASS

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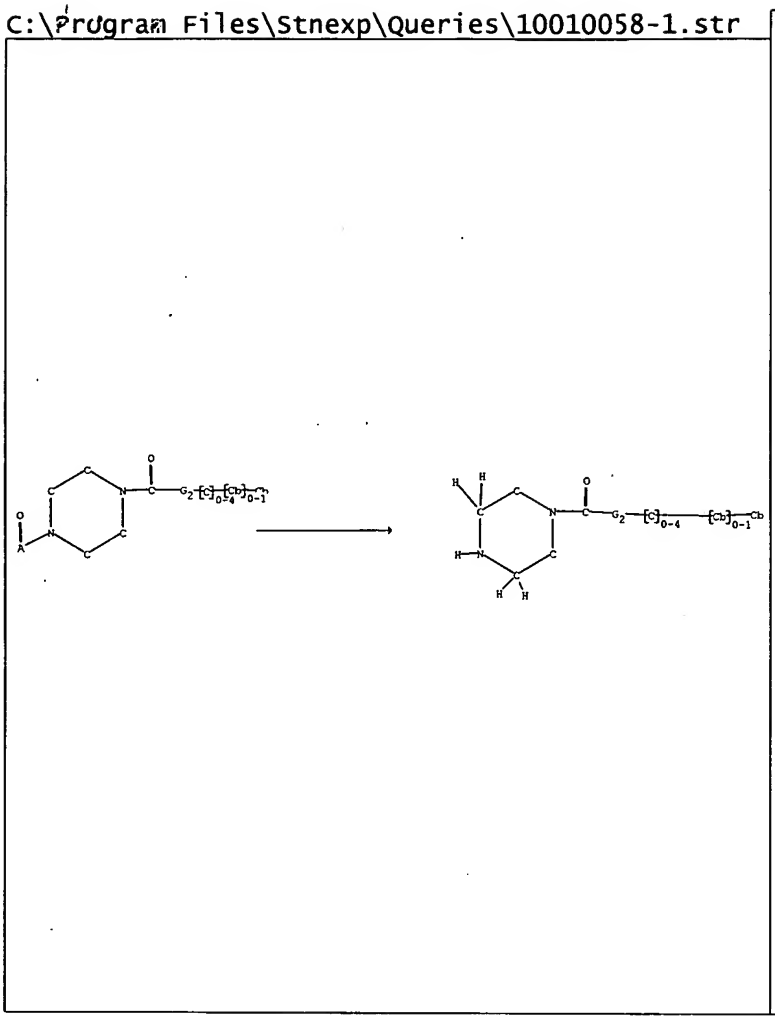

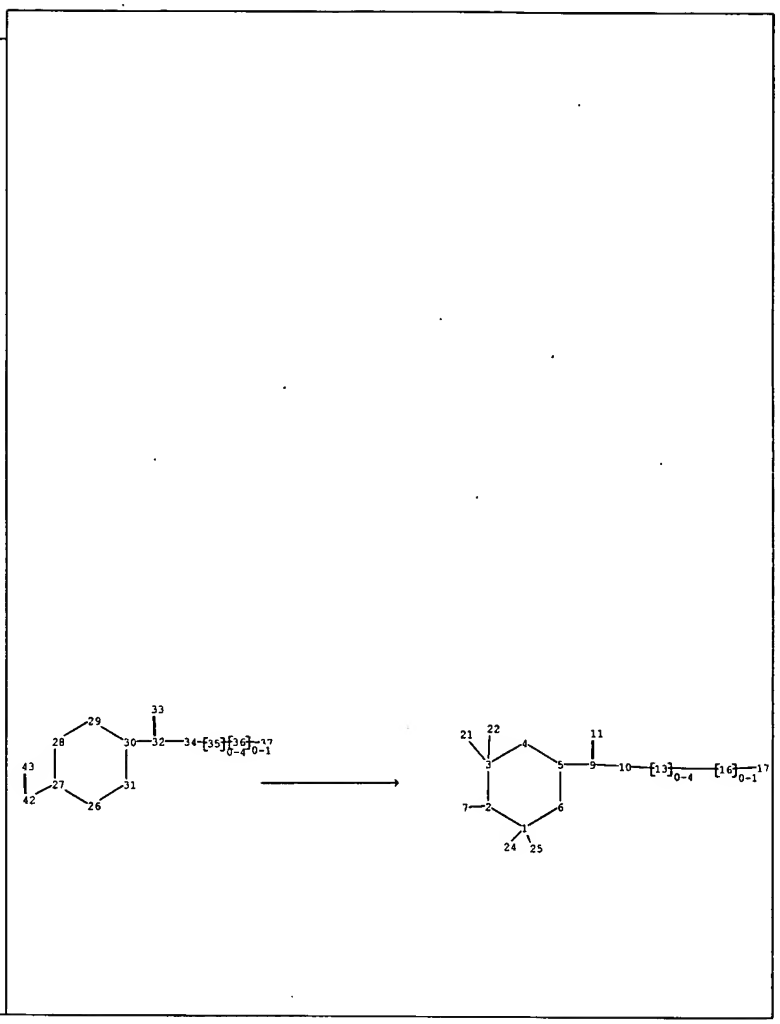

chain nodes :
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ring nodes :
1 2 3 4 5 6 26 27 28 29 30 31
chain bonds :
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32-34 34-35 35-36 36-37 42-43
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 26-27 26-31 27-28 28-29 29-30 30-31
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-9 9-10 9-11 10-13 26-27 26-31 27-28 27-42 28-29
29-30 30-31 30-32 32-33 32-34 34-35 42-43
exact bonds :
1-24 1-25 2-7 3-21 3-22 13-16 16-17 35-36 36-37
isolated ring systems :
containing 1 :

G1:H,CH3

G2:O,S

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 9:CLASS 10:CLASS 11:CLASS
13:CLASS 16:Atom 17:Atom 21:CLASS 22:CLASS 24:CLASS 25:CLASS 26:Atom 27:Atom
28:Atom 29:Atom 30:Atom 31:Atom 32:CLASS 33:CLASS 34:CLASS 35:CLASS 36:Atom
37:Atom 42:CLASS 43:CLASS
fragments assigned product role:
containing 1
fragments assigned reactant/reagent role:
containing 26

10/010058

L6 STRUCTURE UPLOADED

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SCREENING COMPLETE - 154 REACTIONS TO VERIFY FROM 25 DOCUMENTS

100.0% DONE 154 VERIFIED 0 HIT RXNS 0 DOCS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED VERIFICATIONS: 2336 TO 3824
PROJECTED ANSWERS: 0 TO 0

L7 0 SEA SSS SAM L6 (0 REACTIONS)

=> s l6 sss full
FULL SEARCH INITIATED 17:55:47 FILE 'CASREACT'
SCREENING COMPLETE - 4173 REACTIONS TO VERIFY FROM 579 DOCUMENTS

100.0% DONE 4173 VERIFIED 8 HIT RXNS 4 DOCS
SEARCH TIME: 00.00.01

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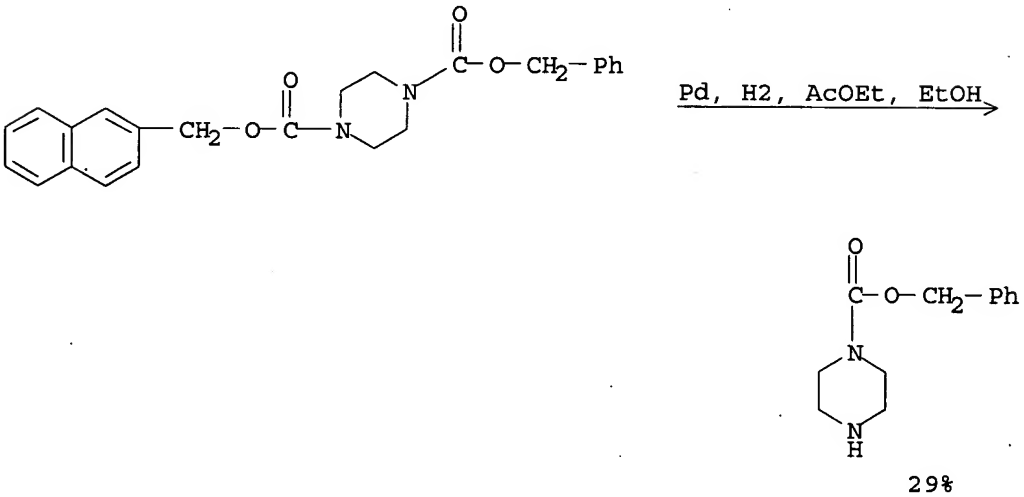
=> d crd

L8 ANSWER 1 OF 4 CASREACT COPYRIGHT 2003 ACS

RX(2) OF 13



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FILE COPY

AN 1994:482867 CAPLUS
DN 121:82867
TI Preparation of carbapenem derivative as antibacterial agent and its intermediate
IN Ishida, Yohei; Saito, Takashi; Nishi, Toshuki; Hayano, Takeshi
PA Daiichi Seiyaku Co, Japan
SO Jpn. Kokai Tokkyo Koho, 14 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 06016671	A2	19940125	JP 1992-173194	19920630
	JP 3040600	B2	20000515		
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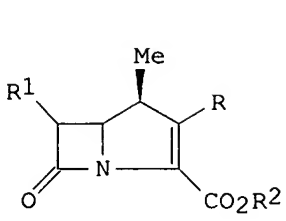
OS CASREACT 121:82867; MARPAT 121:82867
GI

Page 479



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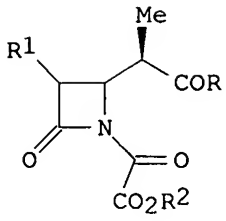

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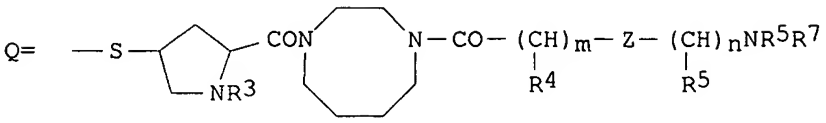
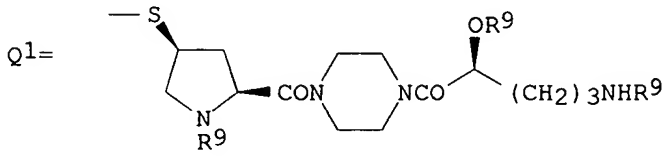


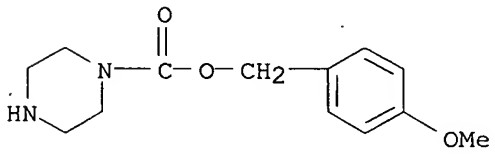


AB The title compds. [I; R = Q; R1 = alkyl, (un)protected hydroxyalkyl; R2 = H, HO2C-protective group; R3, R6, R7 = H, alkyl, protective group; R4 = H, alkyl, halo, (un)protected OH or hydroxyalkyl; R5 = H, alkyl, halo, (un)protected OH, CO2H, or hydroxyalkyl; Z = CH2, O, S, NHCO, CONH; m, n = 0-4], useful as antibacterial agents with excellent in vivo stability and antibacterial activity (no data) are prepd. by cyclization of N-(allyloxalyl)[(pyrrolidinylthio)carbonyl]azetidine derivs. (II; R = Q; R1 - R7, Z, m, n = same as above) with P(R8)3 (R8 = alkoxy, aryloxy, dialkylamino). This process is simple and inexpensive and gives .beta.-lactams of high purity. Thus, a soln. 0.09 mL P(OEt)3 in xylene was added dropwise to a soln. of azetidinone deriv. II [R = Q1, R1 = (R)-MeCHOR9, R9 = allyloxycarbonyl, R2 = allyl] in xylene under refluxing and the refluxing was continued for addnl 16 h to give carbapenem deriv. I [R = Q1, R1 = (R)-MeCHOR9, R9 = allyloxycarbonyl, R2 = allyl] which was dissolved in CH2Cl2 and stirred with [Ph3P]4Pd(0), Bu3SnH, 1 N aq. HCl, and H2O under Ar to give I [R = Q1, R1 = (R)-MeCHOH, R2 = R9 = H].

IT **131004-30-3**, 1-(p-Methoxybenzyloxycarbonyl)piperazine
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with hydroxyproline benzotriazolyl ester deriv.)

RN 131004-30-3 CAPLUS

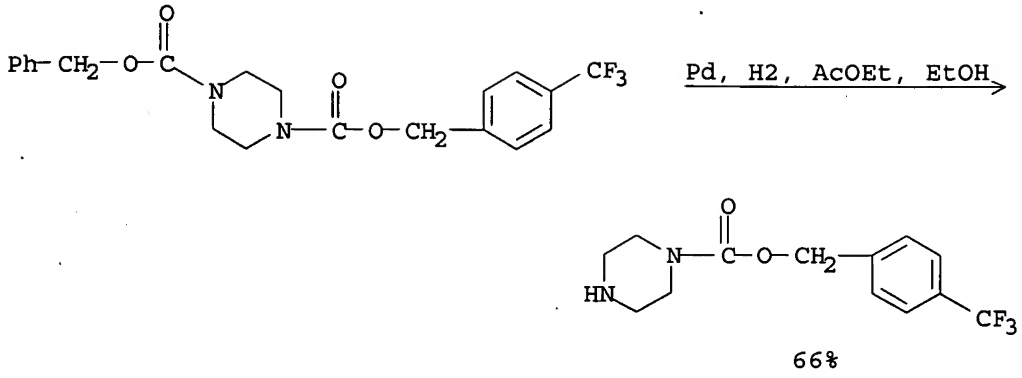
CN 1-Piperazinecarboxylic acid, (4-methoxyphenyl)methyl ester (9CI) (CA INDEX NAME)



L18 ANSWER 148 OF 219 CAPLUS COPYRIGHT 2003 ACS

AN 1994:404529 CAPLUS

RX(3) OF 13



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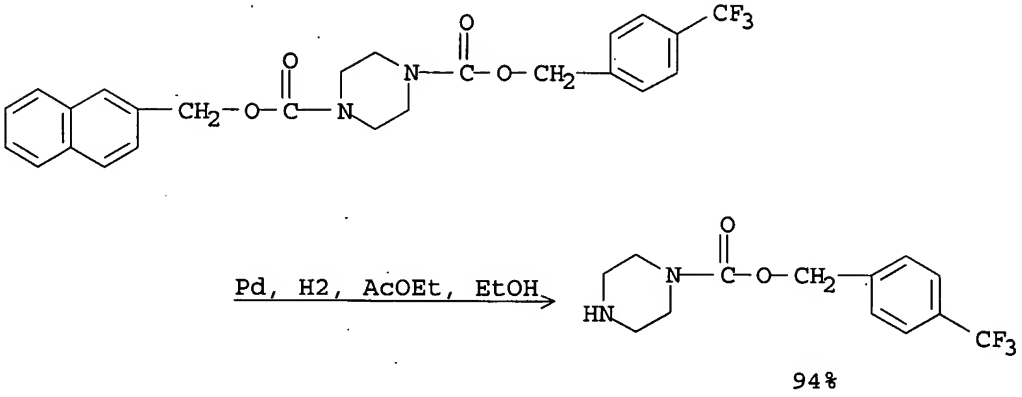

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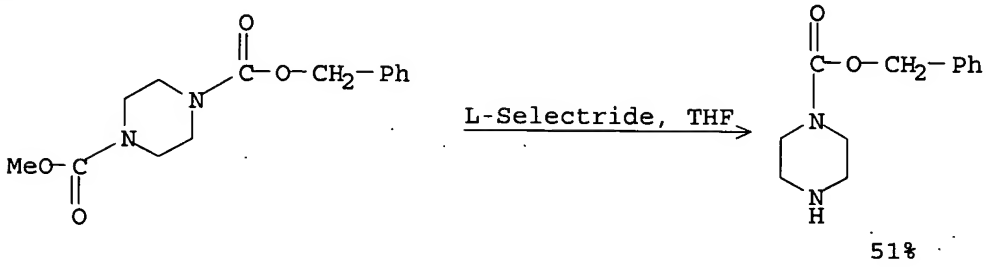
L8 ANSWER 2 OF 4 CASREACT COPYRIGHT 2003 ACS

RX(6) OF 9



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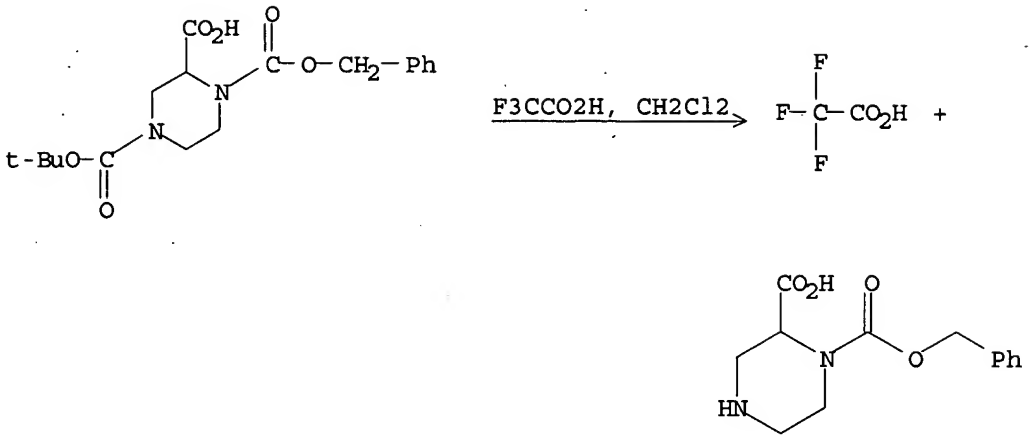
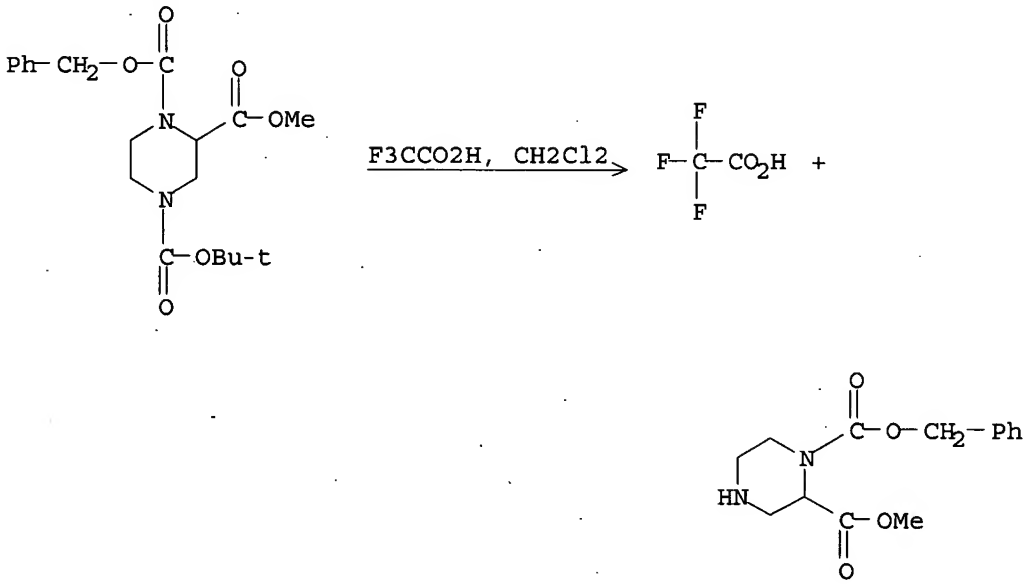
L8 ANSWER 3 OF 4 CASREACT COPYRIGHT 2003 ACS

RX(1) OF 5

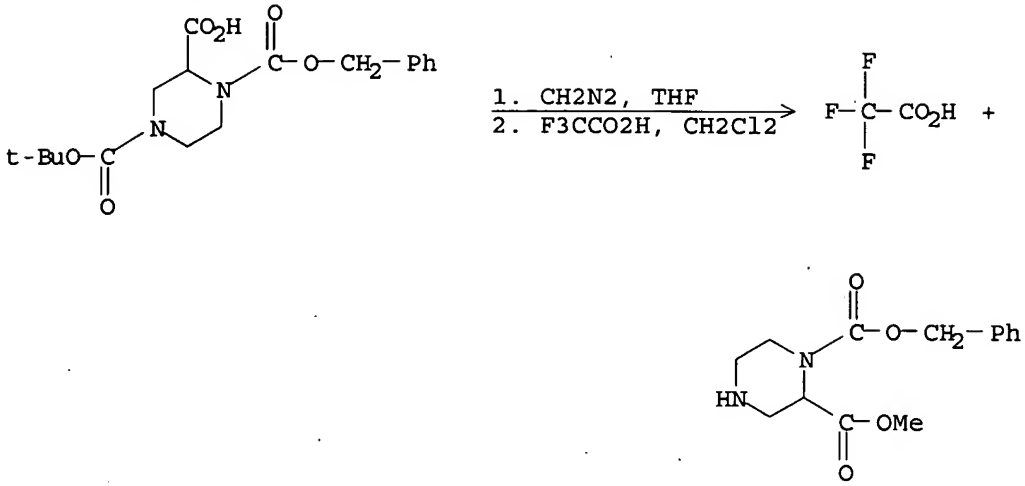


L8 ANSWER 4 OF 4 CASREACT COPYRIGHT 2003 ACS

RX(4) OF 26



RX(11) OF 26 - 2 STEPS



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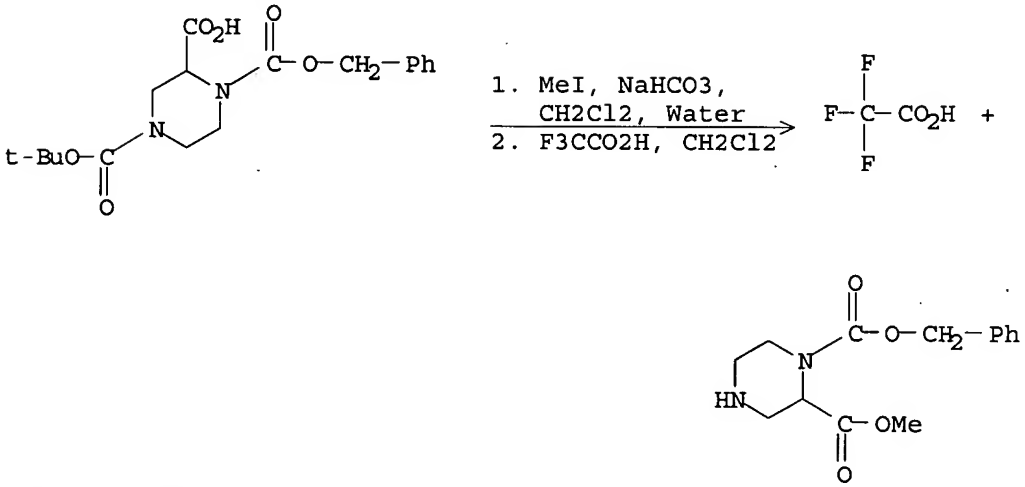
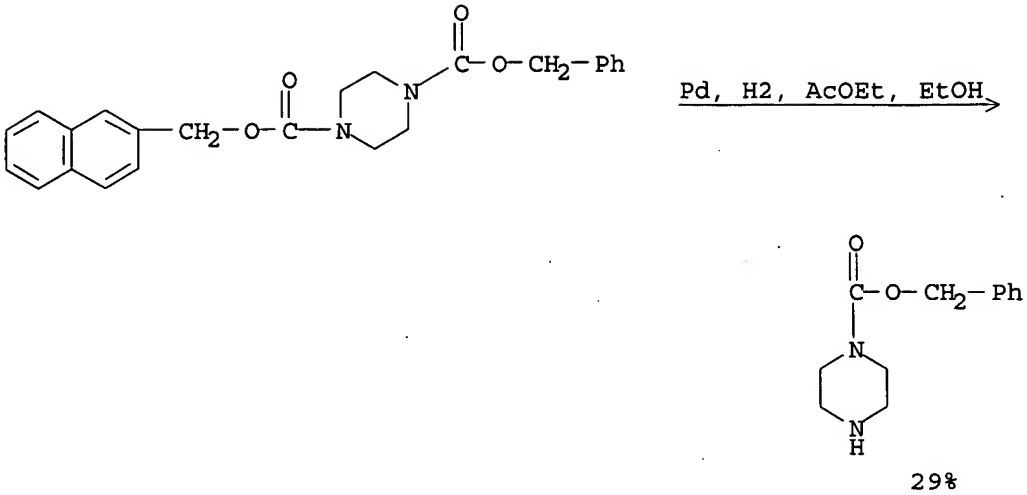


NOTE: 1) Adogen 464 present

=> d 1-4 crdref abs

L8 ANSWER 1 OF 4 CASREACT COPYRIGHT 2003 ACS

RX(2) OF 13



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REF: Organic Letters, 2(8), 1049-1051; 2000

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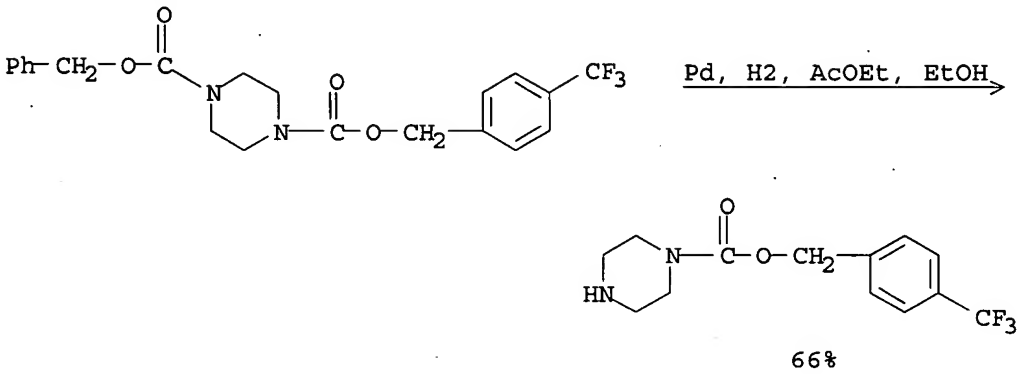

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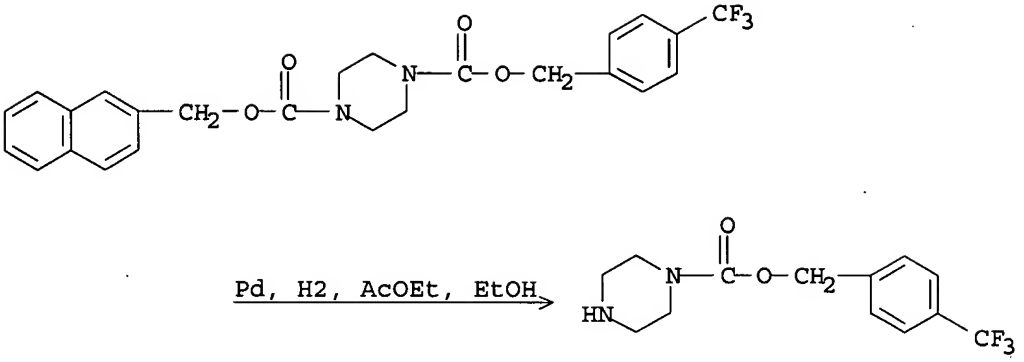
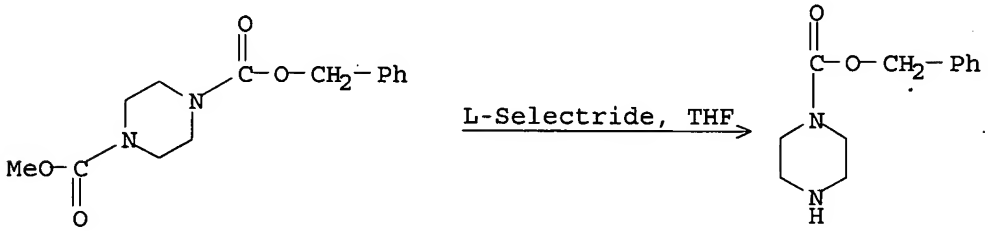


REF: Organic Letters, 2(8), 1049-1051; 2000

AB Highly efficient and selective hydrogenolysis of the 2-naphthylmethyl carbamate group (CNAP) in the presence of the 4-trifluoromethylbenzyl carbamate group (CTFB) has been obsd. for a wide range of substrates. For example, the selective hydrogenolysis of 1,3-phenylenebis[carbamic acid] 1-(2-naphthalenylmethyl) 3-[4-(trifluoromethyl)phenyl]methyl ester in the presence of 10% Pd/C in hydrogen-satd. Et acetate-ethanol for 30 min. gave (3-aminophenyl)carbamic acid [4-(trifluoromethyl)phenyl]methyl ester in 97% yield. The CFTB group is removable by hydrogenation over either 60 mg/mmol substrate of 10% Pd/C or with 20 mg/mmol substrate 20% Pd(OH)2 (Pearlman's catalyst).

L8 ANSWER 2 OF 4 CASREACT COPYRIGHT 2003 ACS

RX(6) OF 9

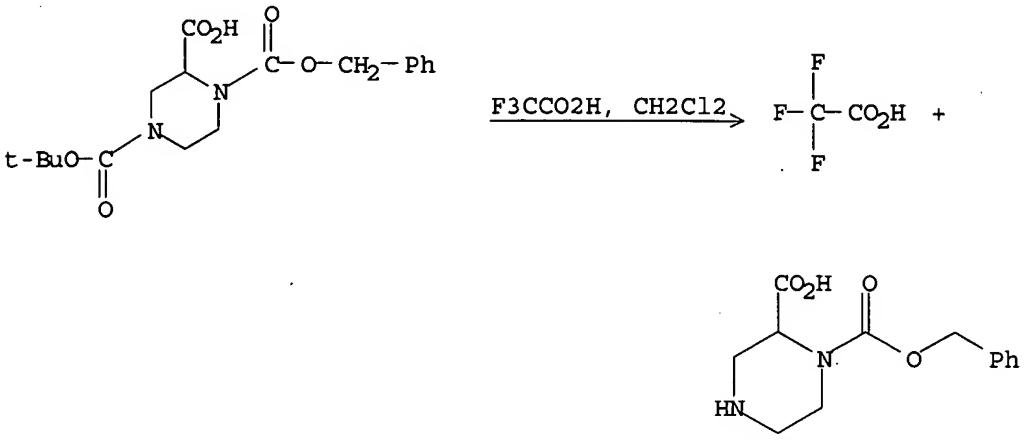


REF: Tetrahedron Letters, 39(49), 8933-8934; 1998

AB L-Selectride selectively cleaves Me carbamates in the presence of more sterically demanding carbamates, including the selective cleavage of a Me carbamate in the presence of an N-Boc group.

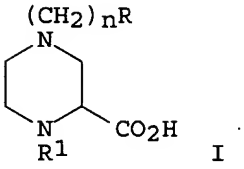
L8 ANSWER 3 OF 4 CASREACT COPYRIGHT 2003 ACS

RX(1) OF 5



REF: Journal of Medicinal Chemistry, 33(10), 2916-24; 1990

GI

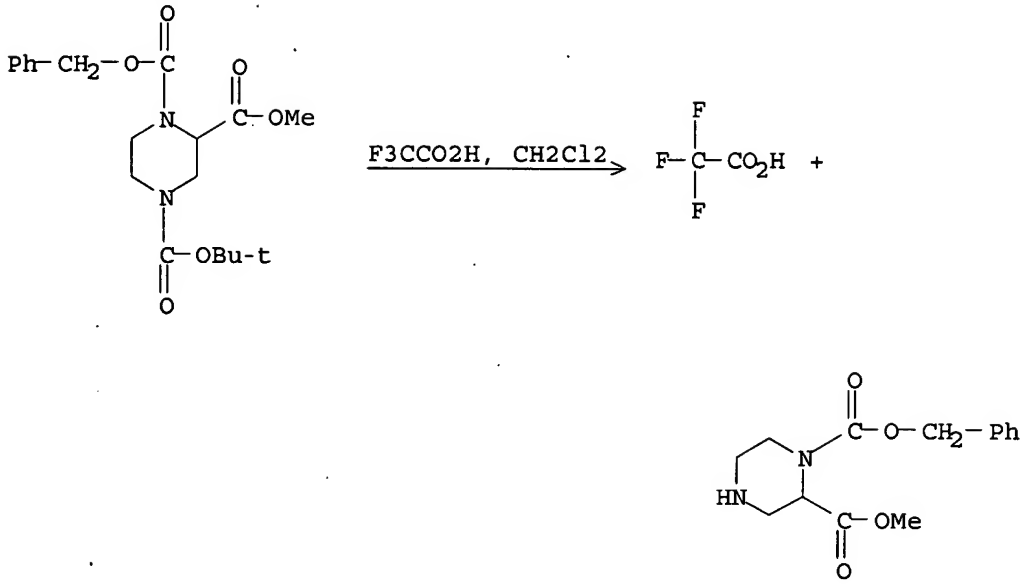


I

AB Fourteen new CPP analogs I [n = 1,3, R = CO2H; n = 2,4, R = PO2H2; n = 1, R = C6H4CH2PO3H2-3; n = 0, R = 2- or 3-H2O2PC6H4, CHPhPO3H2, COC6H4CO2H-2; R1 = H; n = 2, R = PO3H2, R1 = Me, (CH2)3CHPh2, (CH2)2CHPh2, (CH2)3Ph, (CH2)2CH:CPh2] have been prepd. via protected (.+-.)-2-piperazinecarboxylate derivs. I were evaluated as N-methyl-D-aspartate (NMDA) ligands by their ability to displace tritiated I (n = 3, R = PO3H2, R1 = H) from rat cortical membranes. The binding affinity of various chain lengths at N4 of I mimics the binding affinity obsd. for the acyclic derivs. H2O3P(CH2)mCH(NH2)CO2H (m = 2, 4, 6). Analog I (n = 1, R = PO3H2, R1 = H), with a single methylene group in its phosphonate side chain, exhibited diminished affinity for the NMDA receptor when compared to the structurally similar piperidine compd. CGS 19755. Replacement of the phosphonic acid moiety with monoionizable acidic groups such as a carboxylate or a phosphinate resulted in a redn. of binding affinity. An aryl spacer between N4 and the distal acidic group was detrimental to binding, as was alkylation at N1. Steric bulk, however, was better tolerated when a Ph group was positioned .alpha. to the phosphonate, as seen with analogs I (n = 0, R = CHPhPO3H2, R1 = H).

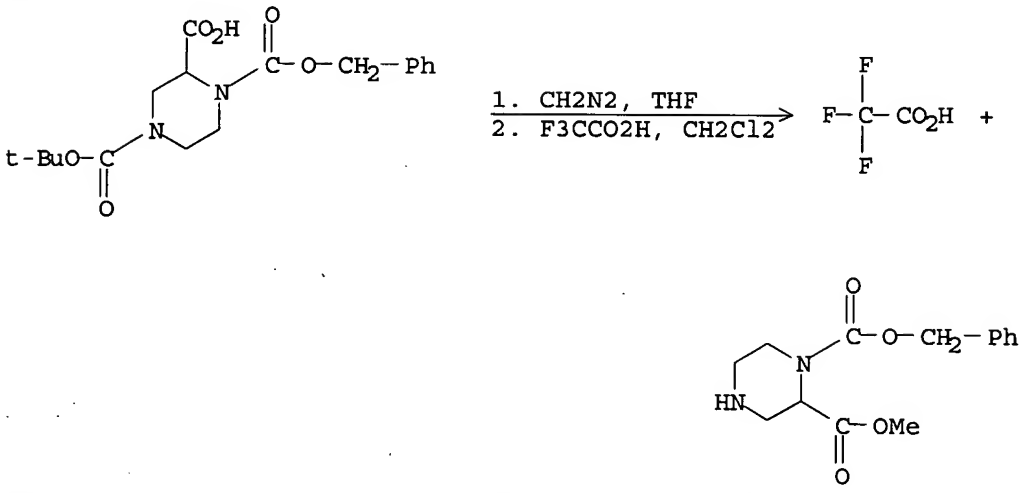
L8 ANSWER 4 OF 4 CASREACT COPYRIGHT 2003 ACS

RX(4) OF 26



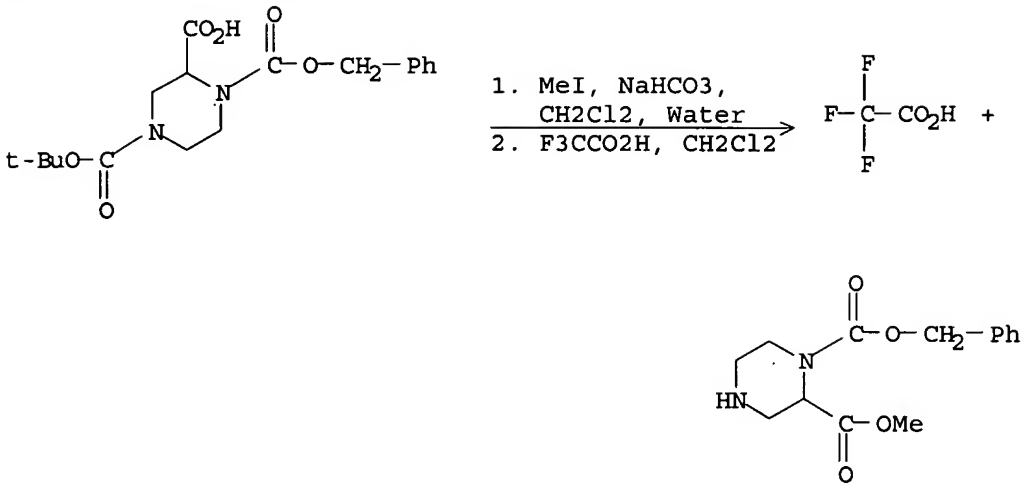
REF: Tetrahedron Letters, 30(39), 5193-6; 1989

RX(11) OF 26 - 2 STEPS



REF: Tetrahedron Letters, 30(39), 5193-6; 1989

RX(12) OF 26 - 2 STEPS



REF: Tetrahedron Letters, 30(39), 5193-6; 1989
NOTE: 1) Adogen 464 present

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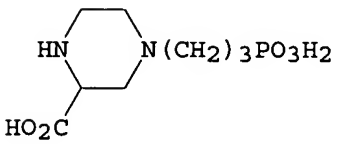

I

AB Two new methods to ensure selective alkylation at N-4 of 2-piperazinecarboxylic acid to give 4-(3-phosphonopropyl)-2-piperazinecarboxylic acid (I) are reported. I was conveniently prepd. using a copper chelate to selectively protect the N-1 position during alkylation. A second procedure used methyl-4-BOC-1-CBZ-2-piperazinecarboxylate as a versatile intermediate, which was further elaborated to give I.

=>

DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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	EP 518558	B1	19980902		
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OS MARPAT 118:233765
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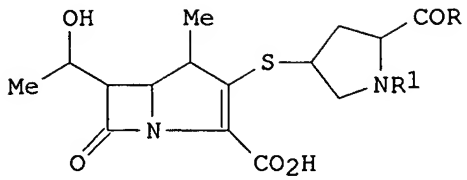

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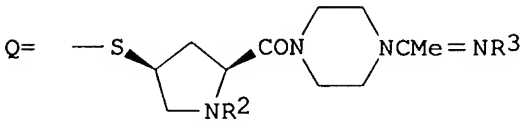
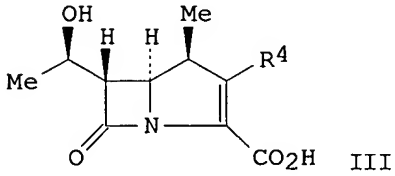




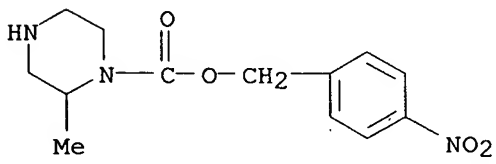
III

AB Title compds. [I; R = N-contg. heterocyclyl(amino), [[(1-iminoalkyl)amino]alkylamino], etc.; R1 = H, alkyl, alkenyl, 1-iminoalkyl, etc.] were prepd. as antibiotics (no data). Thus, (2S,4S)-4-(4-methoxybenzylthio)-1-(4-nitrobenzyloxycarbonyl)-2-pyrrolidinecarboxylic acid was condensed with 1-(tert-butoxycarbonyl)piperazine and the product converted in 3 steps to mercaptopyrrolidinecarboxylate QH [R2 = R3 = CO2CH2C6H4(NO2)-4] (II). 4-Nitrobenzyl (1R, 5R, 6S)-6-[(1R)-1-hydroxyethyl]-1-methyl-2-oxocarbapenam-3-carboxylate was treated with Ph2POCl and (Me2CH)2NEt in MeCN followed by addn. of II to give, after deprotection, title compd. III (R4 = Q, R2 = R3 = H).

IT **147081-26-3 147081-33-2 147081-35-4**
147081-37-6 147081-62-7 147081-74-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in prepn. of antibiotics)

RN 147081-26-3 CAPLUS

CN 1-Piperazinecarboxylic acid, 2-methyl-, (4-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)

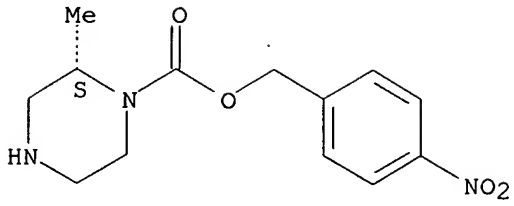


excluded

RN 147081-33-2 CAPLUS

CN 1-Piperazinecarboxylic acid, 2-methyl-, (4-nitrophenyl)methyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

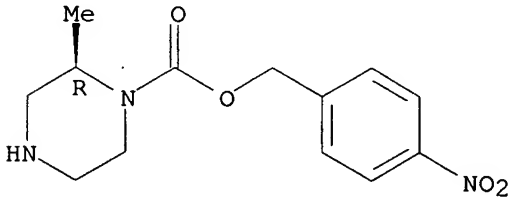


excluded

RN 147081-35-4 CAPLUS
CN 1-Piperazinecarboxylic acid, 2-methyl-, (4-nitrophenyl)methyl ester, (R)- (9CI) (CA INDEX NAME)

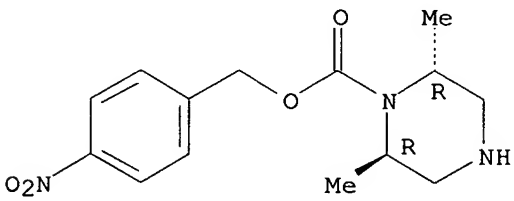
Absolute stereochemistry.

11

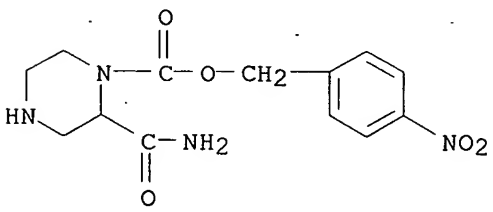


RN 147081-37-6 CAPLUS
CN 1-Piperazinecarboxylic acid, 2,6-dimethyl-, (4-nitrophenyl)methyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 147081-62-7 CAPLUS
CN 1-Piperazinecarboxylic acid, 2-(aminocarbonyl)-, (4-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)



RN 147081-74-1 CAPLUS
CN 1,2-Piperazinedicarboxylic acid, bis[(4-nitrophenyl)methyl] ester (9CI) (CA INDEX NAME)